

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 4.64e-16 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 4.69e-01

**Confidence level:** 5.70e-01

## Nearest Neighbors from the Training Set

Image not found

Oxetane, hexafluoro-

**Measured:** 2.00e-16

**Predicted:** 2.69e-16

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Perfluorotriethylamine

**Measured:** 6.00e-16

**Predicted:** 6.45e-16

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1,2-Dibromo-1,1,2,2-tetrafluoroethane

**Measured:** 1.30e-16

**Predicted:** 2.57e-16

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1,1,1,2,3,3,3-heptafluoropropane

**Measured:** 1.62e-15

**Predicted:** 2.76e-15

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Pentafluoroethane

**Measured:** 2.50e-15

**Predicted:** 2.22e-15